Carbamic acid, ethyl-, methyl ester 6135-31-5 | DTXSID80210261

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 4.58

Global applicability domain: Inside

Local applicability domain index: 9.42e-01

Confidence level: 5.73e-01

Nearest Neighbors from the Training Set

Image not found

1-Hexanol Measured: 5.18 Predicted: 4.67 Image not found

Dipropylamine Measured: 3.59 Predicted: 4.37 Image not found

Cyclohexanol Measured: 5.18 Predicted: 4.72

Image not found

Piperidine Measured: 4.04 Predicted: 4.32 Image not found

1-Pentanol Measured: 4.69 Predicted: 4.17